10/561,031

olicies apply.

They are available for your review at:

http://www.cas.org/legal/infopolicy.html

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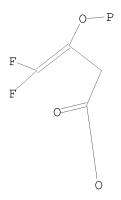
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L5 STRUCTURE UPLOADED

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L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15 full

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 13:58:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 36 TO ITERATE

100.0% PROCESSED 36 ITERATIONS

RATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

L6 1 SEA SSS FUL L5

L7 1 L6

=> d ibib abs hitstr

L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

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ACCESSION NUMBER: 2005:29299 CAPLUS
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DOCUMENT NUMBER: 142:113615

TITLE: Three-step method for producing alkyl

4,4-difluoroacetoacetate esters

APPLICATION NO.

DATE

INVENTOR(S): Gallenkamp, Bernd; Mulder, Lubbertus

PATENT ASSIGNEE(S): Bayer Cropscience Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2

KIND DATE

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

ΙT

RN

CN

823234-80-6P

esters)

(Reactant or reagent)

823234-80-6 CAPLUS

PATENT NO.

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                                                                                  _____
      WO 2005003077
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                              A 20060802 CN 2004-80018512
      CN 1812959
                                                                                    20040618
      JP 2007506673
                               T
                                       20070322 JP 2006-518011
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      US 20060149091
                               A1 20060706 US 2005-561031
                                                                                    20051216
      IN 2005DN05898
                               A
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                                                       IN 2005-DN5898
                                                                                    20051219
PRIORITY APPLN. INFO.:
                                                       DE 2003-10329450 A 20030701
                                                       DE 2003-10331496 A 20030711
                                                       WO 2004-EP6607
                                                                              W 20040618
OTHER SOURCE(S):
                              CASREACT 142:113615; MARPAT 142:113615
      Alkyl difluoroacetoacetate esters (e.g., Et 4,4-difluoroacetoacetate) are
      prepared by: (A) a reaction of alkyl 4-chloro-4,4-difluoroacetoacetates
      (e.g., Et 4-chloro-4,4-difluoroacetoacetate) with trialkyl phosphites
      P(OR1)3 (R1 = C1-4 alkyl; e.g., tri-Me phosphite) giving phosphate esters
      F2C:C[OP(:O)(OR1)2]CH2CO2R[R = alkyl; e.g., Et
      3-[(dimethoxyphosphoryl)oxy]-4,4-difluorobut-3-enoate]; (B) the step (A)
      phosphate esters are reacted with an amine HN(R2)R3 (R2, R3 = H, C1-4
      alkyl; e.g., diisopropylamine) to give enamines F2C:C[N(R2)R3]CH2CO2R
```

(e.g., aqueous HCl) hydrolysis of the step (B) enamines.

[e.g., Et 3-(diisopropylamino)-4,4-difluorobut-3-enoate]; and (C) acid

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(in a three-step method for producing alkyl 4,4-difluoroacetoacetate

3-Butenoic acid, 3-[(dimethoxyphosphinyl)oxy]-4,4-difluoro-, ethyl ester

10/923,271

(CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

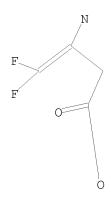
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Uploading C:\Program Files\Stnexp\Queries\10561031d.str

L8 STRUCTURE UPLOADED

=> d

L8 HAS NO ANSWERS L8 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 16 full L9 1 L6

=> d ibib abs hitstr

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:29299 CAPLUS

DOCUMENT NUMBER: 142:113615

TITLE: Three-step method for producing alkyl

4,4-difluoroacetoacetate esters

INVENTOR(S): Gallenkamp, Bernd; Mulder, Lubbertus

PATENT ASSIGNEE(S): Bayer Cropscience Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NΙ,
			NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
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OTHER SOURCE(S): CASREACT 142:113615; MARPAT 142:113615

Alkyl difluoroacetoacetate esters (e.g., Et 4,4-difluoroacetoacetate) are prepared by: (A) a reaction of alkyl 4-chloro-4,4-difluoroacetoacetates (e.g., Et 4-chloro-4,4-difluoroacetoacetate) with trialkyl phosphites P(OR1)3 (R1 = C1-4 alkyl; e.g., tri-Me phosphite) giving phosphate esters F2C:C[OP(:O)(OR1)2]CH2CO2R [R = alkyl; e.g., Et 3-[(dimethoxyphosphoryl)oxy]-4,4-difluorobut-3-enoate]; (B) the step (A) phosphate esters are reacted with an amine HN(R2)R3 (R2, R3 = H, C1-4 alkyl; e.g., diisopropylamine) to give enamines F2C:C[N(R2)R3]CH2CO2R [e.g., Et 3-(diisopropylamino)-4,4-difluorobut-3-enoate]; and (C) acid (e.g., aqueous HC1) hydrolysis of the step (B) enamines.

IT 823234-80-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in a three-step method for producing alkyl 4,4-difluoroacetoacetate esters)

RN 823234-80-6 CAPLUS

CN 3-Butenoic acid, 3-[(dimethoxyphosphinyl)oxy]-4,4-difluoro-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 19 ibib abs hitstr

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:29299 CAPLUS

DOCUMENT NUMBER: 142:113615

TITLE: Three-step method for producing alkyl

4,4-difluoroacetoacetate esters

INVENTOR(S): Gallenkamp, Bernd; Mulder, Lubbertus

PATENT ASSIGNEE(S): Bayer Cropscience Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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APPLICATION NO.
    PATENT NO.
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                                        DE 2003-10329450 A 20030701
PRIORITY APPLN. INFO.:
                                                         A 20030711
                                        DE 2003-10331496
                                        WO 2004-EP6607
                                                           W 20040618
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OTHER SOURCE(S): CASREACT 142:113615; MARPAT 142:113615

Alkyl difluoroacetoacetate esters (e.g., Et 4,4-difluoroacetoacetate) are prepared by: (A) a reaction of alkyl 4-chloro-4,4-difluoroacetoacetates (e.g., Et 4-chloro-4,4-difluoroacetoacetate) with trialkyl phosphites P(OR1)3 (R1 = C1-4 alkyl; e.g., tri-Me phosphite) giving phosphate esters F2C:C[OP(:O)(OR1)2]CH2CO2R [R = alkyl; e.g., Et 3-[(dimethoxyphosphoryl)oxy]-4,4-difluorobut-3-enoate]; (B) the step (A) phosphate esters are reacted with an amine HN(R2)R3 (R2, R3 = H, C1-4 alkyl; e.g., diisopropylamine) to give enamines F2C:C[N(R2)R3]CH2CO2R [e.g., Et 3-(diisopropylamino)-4,4-difluorobut-3-enoate]; and (C) acid (e.g., aqueous HCl) hydrolysis of the step (B) enamines.

10/923,271

IT 823234-80-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in a three-step method for producing alkyl 4,4-difluoroacetoacetate

esters)

RN 823234-80-6 CAPLUS

CN 3-Butenoic acid, 3-[(dimethoxyphosphinyl)oxy]-4,4-difluoro-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s 18 full

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 14:01:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 42 TO ITERATE

100.0% PROCESSED 42 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

L10 2 SEA SSS FUL L8

L11 2 L10

=> d 1-2 ibib abs hitstr

L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:29299 CAPLUS

DOCUMENT NUMBER: 142:113615

TITLE: Three-step method for producing alkyl

4,4-difluoroacetoacetate esters

INVENTOR(S): Gallenkamp, Bernd; Mulder, Lubbertus

PATENT ASSIGNEE(S): Bayer Cropscience Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PA:	CENT :	NO.			KIND DATE			APPLICATION NO.						DATE					
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		JS 20060149091 A1 20060706 US 2005-5610										20040618 20051216								
															20051210					
IN 2005DN05898 A 20070824 IN 2005-DN5898 20051 PRIORITY APPLN. INFO.: DE 2003-10329450 A 20030																				
DE 2003-10329430 A 20030701 DE 2003-10331496 A 20030711																				
	WO 2004-EP6607 W 20040618																			
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AB	Al	kyl d	iflu	oroa	ceto	acet	ate	este:	rs (e.g.	, Et	4,4	-dif	luor	oace	toac	etat	e) are		
	prepared by: (A) a reaction of alkyl 4-chloro-4,4-difluoroacetoacetates (e.g., Et 4-chloro-4,4-difluoroacetoacetate) with trialkyl phosphites																			
	P(OR1)3 (R1 = C1-4 alkyl; e.g., tri-Me phosphite) giving phosphate esters $F2C:C[OP(:O)(OR1)2]CH2CO2R$ [R = alkyl; e.g., Et														esters					
	F20	C:C[O	P(:0) (OR	1)2]	CH2C	02R	[R =	alk	yl;	e.g.	, Et		. 7						
																		p (A)		
	_	ospha cyl;															•			
		.g.,																		
		.g.,														πα (c, a	Ciu		
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					nt);	SPN	(Sy	nthe	tic ¡	orep	arat	ion)	; PR	EP (Prep	arat	ion)	; RACT		
		eacta													-					
		(in	a th	ree-	step	met]	hod	for :	prod	ucin	g al	kyl	4,4-	difl	uoro	acet	oace	tate		
		este.																		
RN		3234-															,			

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(CA INDEX NAME)

CN

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

3-Butenoic acid, 3-[bis(1-methylethyl)amino]-4,4-difluoro-, ethyl ester

L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:309977 CAPLUS

DOCUMENT NUMBER: 125:87124

ORIGINAL REFERENCE NO.: 125:16457a, 16460a

TITLE: Biomimetic base-catalyzed [1,3]-proton shift reaction.

A practical synthesis of β -fluoroalkyl- β -amino acids

AUTHOR(S): Soloshonok, Vadim A.; Kukhar, Valery P.

CORPORATE SOURCE: Natl. Inst. Res., Inst. Nagoya, Nagoya City, 462,

Japan

SOURCE: Tetrahedron (1996), 52(20), 6953-6964

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:87124

AB An efficient approach to practical synthesis of $\beta\text{-fluoroalkyl-}\beta\text{-amino}$ acids is described. The method consists in the reducing reagent-free base-catalyzed biomimetic transamination reaction between fluorinated $\beta\text{-keto}$ carboxylic esters and benzylamine. This transformation involves two sequential base-catalyzed [1,3]-proton transfers giving rise to corresponding N-benzylidene derivs. as the products of final thermodn. equilibration, directed by the electron-withdrawing character of fluoroalkyl groups. Opportunity for catalytic enantiocontrolled synthesis of targeted $\beta\text{-amino}$ acids with application of monochiral base, as a catalyst for these isomerizations, is demonstrated.

IT 178381-17-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of fluoroalkyl $\beta\text{-amino}$ acids via isomerization of benzyl enamines)

RN 178381-17-4 CAPLUS

CN 3-Butenoic acid, 4,4-difluoro-3-[(phenylmethylene)amino]-, methyl ester (CA INDEX NAME)